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One-step Taylor–Galerkin methods for convection–diffusion problems

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Abstract

Third and fourth order Taylor–Galerkin schemes have shown to be efficient finite element schemes for the numerical simulation of time-dependent convective transport problems. By contrast, the application of higher-order Taylor–Galerkin schemes to mixed problems describing transient transport by both convection and diffusion appears to be much more difficult. In this paper we develop two new Taylor–Galerkin schemes maintaining the accuracy properties and improving the stability restrictions in convection–diffusion. We also present an efficient algorithm for solving the resulting system of the finite element method. Finally we present two numerical simulations that confirm the properties of the methods.

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1. Introduction

In an attempt to develop efficient finite element schemes for the numerical simulation of time-dependent convective transport problems, Taylor–Galerkin (TG) schemes with third- and fourth order accuracy in the time were developed over the last years and successfully applied in the solution of engineering problems. See for instance references [1,4,3] for an overview of the properties of third and fourth order TG schemes for pure advection.

By contrast, the application of higher-order TG schemes to mixed problems describing transient transport by both convection and diffusion appears to be much more difficult. This is due to the presence of the Laplacian operator in the governing equation which does not allow the TG procedure to be carried out to third or higher order in conjunction with the use of standard C^0 finite elements for spatial discretization. Ref. [2] presents an early study of second-order Taylor–Galerkin schemes for convection–diffusion problems.

2. Time discretization

In order to introduce the second order TG method for evolutionary advection–diffusion problems in the simplest possible way, while retaining all the essential features of the method, we first consider the linear advection–diffusion equation for the scalar quantity u

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$$u_t = -\vec{a} \cdot \nabla u + v \nabla^2 u, \quad (1)$$

where \vec{a} is the advection velocity and $v > 0$ the diffusion coefficient. Both \vec{a} and v are assumed to be constant.

By contrast with the current practice in the finite element solution of initial boundary value problems which consists of performing spatial discretization before time discretization, the reverse is true in the TG approach. In fact, like in the Lax–Wendroff finite difference method, time discretization precedes space discretization in the TG approach.

With the aid of the Taylor series expansion in time of u and using (1) we arrive at the following semi-discrete equation

$$\begin{aligned} u_t^n &= -\vec{a} \cdot \nabla u^n + v \nabla^2 u^n, \\ u_{tt}^n &= (\vec{a} \cdot \nabla)^2 u^n + v \nabla^2 (u_t^n - v \nabla^2 u^n) + v \nabla^2 u_t^n \\ &= (\vec{a} \cdot \nabla)^2 u^n + 2v \nabla^2 \left(\frac{u^{n+1} - u^n}{\Delta t} \right) + \mathcal{O}(\Delta t, v^2). \end{aligned} \quad (2)$$

Now, introducing (2) into the Taylor series expansion in time for u , we obtain the scheme

$$[1 - \Delta t v \nabla^2] \frac{u^{n+1} - u^n}{\Delta t} = -\vec{a} \cdot \nabla u^n + v \nabla^2 u^n + \frac{\Delta t}{2} (\vec{a} \cdot \nabla)^2 u^n. \quad (3)$$

This is a new TG-algorithm (TG2C2D) for convection–diffusion problems. Its global accuracy is $\mathcal{O}(\Delta t^2, v^2 \Delta t)$, but in general it has second order accuracy because usually $v^2 \leq \Delta t$. This method is identical to TG2 (see [1]) for pure convection ($v = 0$). However, it represents a valuable extension of TG2 for convection–diffusion problems because, the new scheme retains the phase accuracy of TG2, but has a better stability when the diffusion dominates the transport process. The scheme (3) has the same drawbacks as TG2 for pure convection in that it has a strong stability restriction and exhibits some numerical dispersion. We can circumvent this problem by incorporating in the scheme a third order approximation of the convective term. This leads to a new improved scheme for convection–diffusion equations (TG3C2D) which reads

$$\left[1 - \frac{\Delta t^2}{6} (\vec{a} \cdot \nabla)^2 - \Delta t v \nabla^2 \right] \frac{u^{n+1} - u^n}{\Delta t} = -\vec{a} \cdot \nabla u^n + v \nabla^2 u^n + \frac{\Delta t}{2} (\vec{a} \cdot \nabla)^2 u^n. \quad (4)$$

The global accuracy of (4) is $\mathcal{O}(\Delta t^3, v^2 \Delta t, v \Delta t^2)$. Usually $v^2 \leq \Delta t$, so the scheme is third order accurate as regards convection and second order accurate for diffusion. If $v \leq \Delta t$ the method is third order accurate. When $v = 0$, TG3C2D reduces to the classical TG3 scheme introduced in [1].

3. Spatial discretization

We apply the Galerkin formulation in space to obtain the fully discrete version of the previous schemes. We use the standard local interpolations with linear or multilinear shape functions. Let Ω denote the domain of the problem, and $\Gamma = \partial\Omega$ its boundary. Denoting $\langle \cdot, \cdot \rangle_\Omega$ the inner product in $L^2(\Omega)$ and $\langle \cdot, \cdot \rangle_\Gamma$ the inner product in $L^2(\Gamma)$, the scheme TG3C2D takes the form

$$\begin{aligned} & \sum_j \left[\langle N_j, N_i \rangle_\Omega + \Delta t v (\langle \nabla N_j, \nabla N_i \rangle_\Omega - \langle \vec{n} \cdot \nabla N_j, N_i \rangle_\Gamma) \right. \\ & \quad \left. + \frac{\Delta t^2}{6} (\langle \vec{a} \cdot \nabla N_j, \vec{a} \cdot \nabla N_i \rangle_\Omega - \langle \vec{a} \cdot \nabla N_j, \vec{a} \cdot \vec{n} N_i \rangle_\Gamma) \right] \frac{(U_j^{n+1} - U_j^n)}{\Delta t} \\ & = \sum_j \left[-\langle \vec{a} \cdot \nabla N_j, N_i \rangle_\Omega U_j^n - v \langle \nabla N_j, \nabla N_i \rangle_\Omega U_j^n \right. \\ & \quad \left. + \frac{\Delta t}{2} (-\langle \vec{a} \cdot \nabla N_j, \vec{a} \cdot \nabla N_i \rangle_\Omega U_j^n + \langle \vec{a} \cdot \nabla N_j, \vec{a} \cdot \vec{n} N_i \rangle_\Gamma U_j^n) + v \langle \vec{n} \cdot \nabla N_j, N_i \rangle_\Gamma U_j^n \right]. \end{aligned} \quad (5)$$

A similar expression is obtained for TG2C2D.

4. Accuracy and stability analysis

If we use piecewise linear basis functions on a uniform mesh, the evolution of a Fourier component can be written in the form

$$U_{r,l}^{n+1} = GU_{r,l}^n, \quad (6)$$

where $U_{r,l}^n = U(x_0 + rh, y_0 + lh, t_0 + n\Delta t)$ and G is the amplification factor, Δt and h are the time and spatial increments, respectively, supposed constant in the mesh. The numerical values of G show good accuracy properties in the frequency range of interest, that is, the frequencies with an acceptable spatial approximation.

The stability limits of schemes TG2C2D and TG3C2D in 1D and 2D are shown in Fig. 1 where $c = |a|\Delta t/h$ is the Courant number in 1D, $d = \nu\Delta t/h^2$ the diffusion number, $\vec{c} = (c_1, c_2) = \vec{a}\Delta t/h$ the Courant vector and $c = \|\vec{c}\|$ the Courant number in 2D.

One notes in Fig. 1 that TG2C2D and TG3C2D improve the stability limit of the usual second-order TG methods and also maintain a good phase accuracy when diffusion increases. For a more complete comparison we also show in Fig. 1 the stability limits of three other explicit methods. The first is a three-stage third-order TG scheme (3TG3) [5,6]. The second is a one-step second-order (for convection) TG scheme (TG2pe) [7,8], while the third method is a two-step

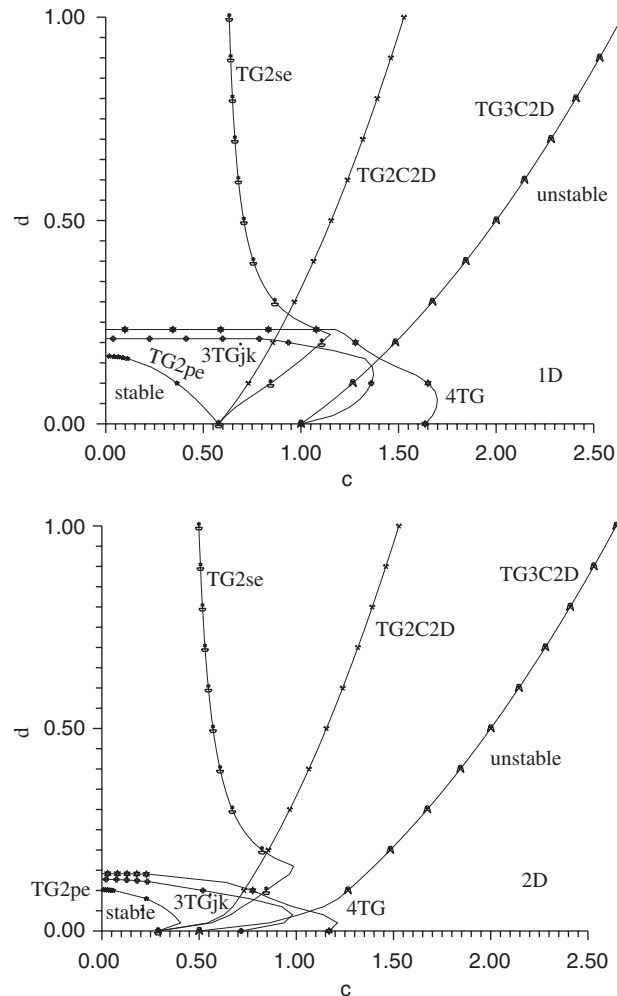


Fig. 1. Stability limits in 1D and 2D.

scheme with operator splitting (TG2se) [10]. Also, these three methods suffer from a reduced accuracy when diffusion is important.

The Fig. 1 show that the developed methods increases the computational efficiency when diffusion appears due to the improved stability limit.

4.1. Numerical optimization

A direct application of the Galerkin approximation in Eq. (5) gives a system of equations where the matrix depend on diffusion in the TG2C2D case, and also it depends on convection in the TG3C2D case. This is a drawback in non linear problems. We can circumvent this drawback with the explicit algorithm proposed in this section.

We decompose the matrix of the resulting finite element system as the usual mass matrix \mathbf{M} , plus another matrix \mathbf{Q} that contains the diffusion and the convection in the TG3C2D case,

$$\left(\mathbf{M} + \frac{\Delta t}{2}\mathbf{Q}\right)\vec{U} = \vec{b}, \quad (7)$$

where \vec{b} is the residual and $\vec{U} = (\vec{u}^{n+1} - \vec{u}^n)/\Delta t$.

Let \vec{y} be the solution of $\mathbf{M}\vec{y} = \vec{b}$. The system (7) can be rearranged as

$$\vec{U} = \left(\mathbf{I} + \frac{\Delta t}{2}\mathbf{M}^{-1}\mathbf{Q}\right)^{-1}\vec{y}. \quad (8)$$

Using $(\mathbf{I} + \mathbf{A})^{-1} = \sum_{k=0}^{\infty} (-1)^k \mathbf{A}^k$ with the notation $\mathbf{A}^0 = \mathbf{I}$, we can obtain

$$\left(\mathbf{I} + \frac{\Delta t}{2}\mathbf{M}^{-1}\mathbf{Q}\right)^{-1} = \mathbf{I} - \frac{\Delta t}{2}\mathbf{M}^{-1}\mathbf{Q} + \frac{\Delta t^2}{4}\mathbf{M}^{-1}\mathbf{Q}\mathbf{M}^{-1}\mathbf{Q} + \mathcal{O}(\Delta t^3), \quad (9)$$

and, subsequently,

$$\begin{aligned} \vec{U} &= \left(\mathbf{I} - \frac{\Delta t}{2}\mathbf{M}^{-1}\mathbf{Q}\right)\vec{y} + \mathcal{O}(\Delta t^2), \\ \vec{U} &= \left(\mathbf{I} - \frac{\Delta t}{2}\mathbf{M}^{-1}\mathbf{Q} + \frac{\Delta t^2}{4}\mathbf{M}^{-1}\mathbf{Q}\mathbf{M}^{-1}\mathbf{Q}\right)\vec{y} + \mathcal{O}(\Delta t^3). \end{aligned} \quad (10)$$

Now using (10) we can solve the system (7) resulting from the finite element formulation with an explicit algorithm of second order in time for TG2C2D:

$$\begin{cases} \mathbf{M}\vec{y} = \vec{b}, \\ \mathbf{M}\vec{U} = \vec{b} - \frac{\Delta t}{2}\mathbf{Q}\vec{y} + \mathcal{O}(\Delta t^2). \end{cases} \quad (11)$$

Similarly, for TG3C2D we can use an explicit scheme of third order in time:

$$\begin{cases} \mathbf{M}\vec{y}_1 = \vec{b}, \\ \mathbf{M}\vec{y}_2 = \vec{b}_1 \quad \text{where } \vec{b}_1 = \mathbf{Q}\vec{y}_1, \\ \mathbf{M}\vec{U} = \vec{b} - \frac{\Delta t}{2}\vec{b}_1 + \frac{\Delta t^2}{4}\mathbf{Q}\vec{y}_2 + \mathcal{O}(\Delta t^3). \end{cases} \quad (12)$$

Using the developed schemes we obtain a significant save in the computational time. This is due because the system matrices are the same and symmetric and only one decomposition is needed.

We have observed that we can *lump* the matrix in the systems in (11) and in (12) except in the last one without apparent changes in precision.

5. Numerical simulations

We have done several numerical simulations that permits to check the properties of the proposed methods and their computational efficiency. First we solve a problem with analytical solution, the evolution of a Gaussian 2D wave by linear convection–diffusion. Afterwards we solve a highly nonlinear problem that simulates the evolution of a water saturated avalanche down hill.

5.1. Convection–diffusion of a 2D Gaussian wave

To illustrate the performance of the developed schemes consider first the linear convection–diffusion problem over the spatial domain $\Omega = [0, 6] \times [0, 6]$ defined by

$$\begin{cases} u_t + \vec{a} \cdot \nabla u = v \nabla^2 u & \text{where } \vec{a} = (a_1, a_2), \\ u(x, y, 0) = \frac{1}{\sigma_0} (e^{-(1/2)(x-x_0)^2/\sigma_0^2} + e^{-(1/2)(y-y_0)^2/\sigma_0^2}) \end{cases} \quad (13)$$

with exact Dirichlet boundary conditions in Γ_{in} and free stress in Γ_{out} where $\partial\Omega = \Gamma_{\text{in}} \cup \Gamma_{\text{out}}$ and $\Gamma_{\text{in}} \cap \Gamma_{\text{out}} = \emptyset$.

This problem has analytical solution defined by

$$u(x, y, t) = \frac{1}{\sigma(t)} \left(e^{-(1/2)(x-x_0-a_1t)^2/\sigma^2(t)} + e^{-(1/2)(y-y_0-a_2t)^2/\sigma^2(t)} \right), \quad (14)$$

where $\sigma(t) = \sigma_0 \sqrt{1 + 2vt/\sigma_0^2}$.

We have used a bilinear uniform mesh of size h and a skewed velocity $\vec{a} = (0.7, 0.7)$ for several values of v . Table 1 shows the global order of the methods that fits with the expected values in (3) and (4).

Fig. 2 shows the numerical solution using the TG3C2D method with a direct solution of the system (7) and with the proposed algorithm (12) with *lumped* matrix except in the last step.

Table 1
Global order of the methods

v	TG2C2D	TG3C2D
0	2.1	3.1
10^{-7}	2.1	3.1
0.01	2.1	2.7
0.1	2.1	2.1

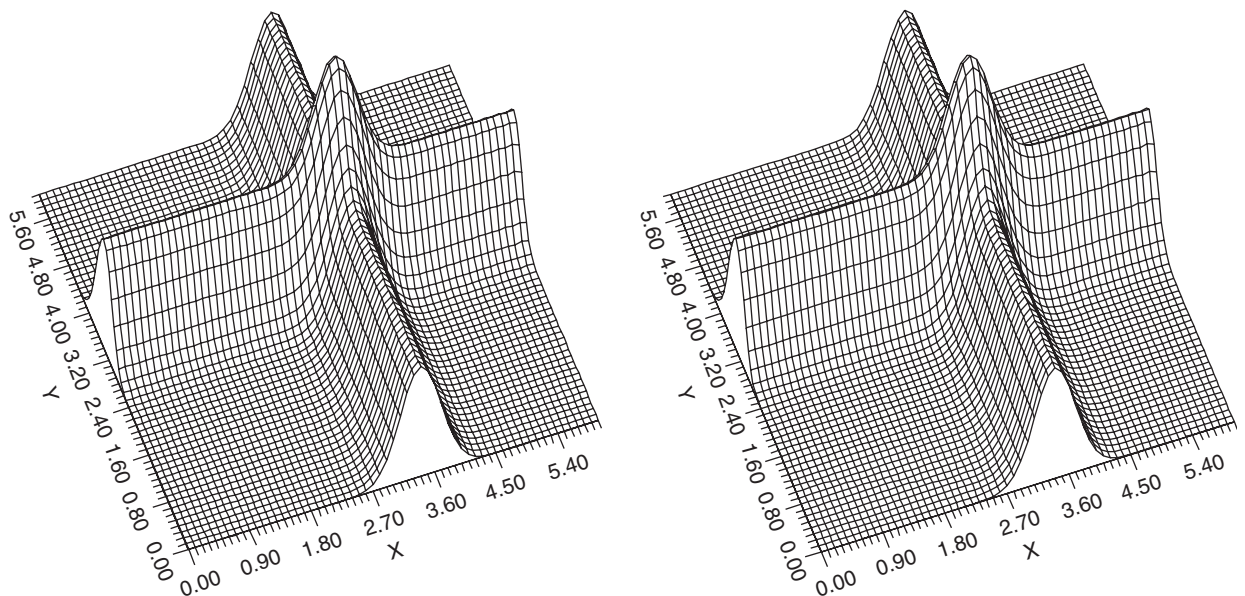


Fig. 2. Convection–diffusion of a Gaussian by TG3C2D with $h = 0.1$ and $v = 10^{-5}$ for $t = 1$ with direct resolution of the system (left) and with the algorithm proposed (right).

5.2. Avalanche simulation

Here we model a water saturated avalanche down hill using two surfaces: the lower one at the base z_b , and the upper one z_s (see Fig. 3). The difference $z_s - z_b$ defines the position of the avalanche at any time.

We assume that we have only the gravity force, and that the material moves as a newtonian fluid. We also assume that there is not erosion and that the material does not slip at the base. Using these assumptions, the displacement of the avalanche is approximated by the equation

$$\frac{\partial z_s}{\partial t} + \frac{\partial}{\partial x} \left[\frac{1}{3\mu} (z_s - z_b)^3 \right] - \frac{\partial}{\partial x} \left[\varphi_x \left(\frac{1}{3\mu} (z_s - z_b)^3 \right) \frac{\partial z_s}{\partial x} \right] - \frac{\partial}{\partial y} \left[\eta \varphi_y \left(\frac{1}{3\mu} (z_s - z_b)^3 \right) \frac{\partial z_s}{\partial y} \right] = 0 \quad (15)$$

where μ is the viscosity of the material [9].

This study is a two-dimensional generalization of [11] where they study the avalanche of the Madison canyon in 1959 caused by an earthquake. We have used several time integration schemes for computing the avalanche evolution from $t = 0$ to $t = 38$ with $\Delta t = 80\%$ of Δt_{\max} (t is the adimensional time). In this problem the explicit time integration schemes has strict stability restrictions on Δt due to the presence of the diffusion operator. Table 2 shows that the TG3C2D scheme is the most efficient in view of the computational time.

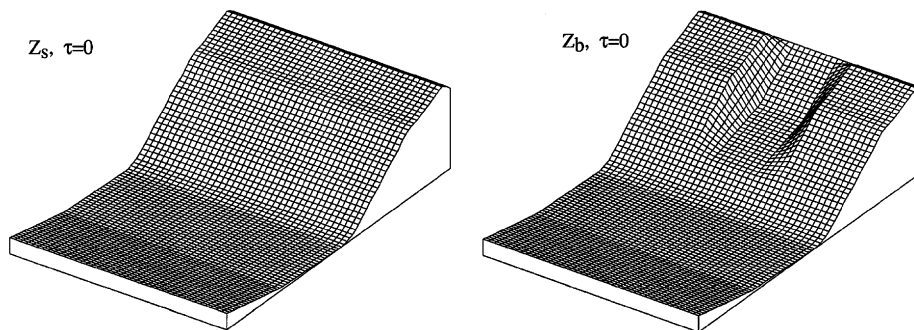


Fig. 3. Initial surfaces z_s (left) and z_b (right) of the avalanche.

Table 2

Computational time for $t = 38$

Method	Steps Δt	CPU (seg.)
3TGjk	1846	1626
TG2Pe	2230	719
TG3C2D	586	566

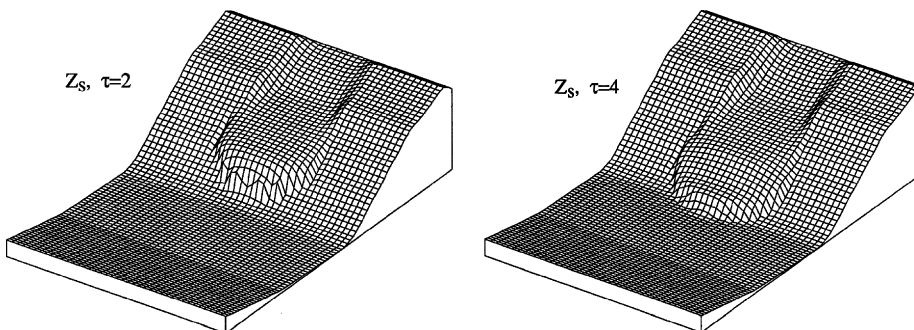


Fig. 4. Avalanche position for $t = 2$ (left) and $t = 4$ (right).

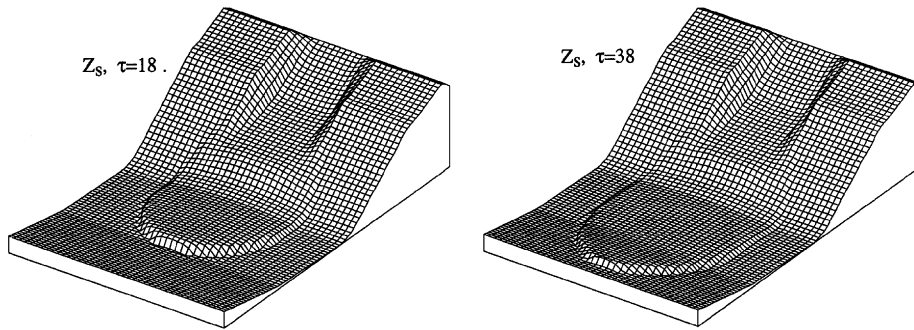


Fig. 5. Avalanche position for $t = 18$ (left) and $t = 38$ (right).

The TG3C2D method remove the spurious oscillations in high gradient regions, that is, in the front of the avalanche (see Figs. 4 and 5). We note that the explicit Taylor–Galerkin methods are not designed for stationary problems.

6. Conclusions

Performing the time discretization before the spatial discretization and using some approximations we have obtained two new TG schemes that maintains the precision in the convection–diffusion case. Although the standard TG schemes suffers of serious stability restrictions in the presence of diffusion, the new developed methods improves the stability region when the diffusion appears.

We have presented an optimization algorithm for solving resulting finite element system without decomposing the matrix at each time step. It is essential in the nonlinear case because the matrix of the system depends on the diffusion in TG2C2D and also on the velocity in TG3C2D.

The numerical results confirm the good mathematical properties of our algorithms. The developed schemes obtain good accuracy solutions without spurious oscillations and computational efficiency.

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